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A Mathematical Framework for Multiscale Science and Engineering:

The Variational Multiscale Method and Interscale Transfer Operators

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April 28, 2004

Abstract

Existing approaches in multiscale science and engineering have evolved from a range of ideas and solutions that are reflective of their original problem domains. As a result, research in multiscale science has followed widely diverse and disjoint paths, which presents a barrier to cross pollination of ideas and application of methods outside their application domains. The status of the research environment calls for an abstract mathematical framework that can provide a common language to formulate and analyze multiscale problems across a range of scientific and engineering disciplines. In such a framework, critical common issues arising in multiscale problems can be identified, explored and characterized in an abstract setting. This type of overarching approach would allow categorization and clarification of existing models and approximations in a landscape of seemingly disjoint, mutually exclusive and *ad hoc* methods. More importantly, such an approach can provide context for both the development of new techniques and their critical examination. As with any new mathematical framework, it is necessary to demonstrate its viability on problems of practical importance. At Sandia, lab-centric, prototype application problems in fluid mechanics, reacting flows, magnetohydrodynamics (MHD), shock hydrodynamics and materials science span an important subset of DOE Office of Science applications and form an ideal proving ground for new approaches in multiscale science. This

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document represents our initial thoughts on developing a mathematical framework for multi-scale applications. As such, we expect that future versions of this document will build upon these ideas.

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A Mathematical Framework for Multiscale Science and Engineering: The Variational Multiscale Method and Interscale Transfer Operators

1 Introduction

Multiple scales co-exist in virtually all science and engineering applications. For some applications, accurate computational modeling is possible by neglecting all but one dominant scale. However, many physical systems of importance to the DOE Office of Science exhibit multiscale behavior that requires resolution of several scales and their concomitant coupled interactions. Such systems are characterized by important coupled multiple length-scales and time-scales that can vary by many orders of magnitude. Examples include turbulent fluid flow and reacting flows, geophysical flow systems, plasma systems that include magnetically-driven coupled plasma-hydrodynamic phenomena, materials science applications such as fracture, and biological systems modeling. Conventional modeling techniques replace small scales by constitutive models and empirical closures that are incapable of capturing the complexity of coupled scale interactions. For these reasons, multiscale approaches to modeling complex physical systems are becoming increasingly important.

In the ensuing discussion, which briefly motivates and describes a mathematical framework for multiscale science, we focus on two main application categories of multiscale problems. The first category includes problems that allow application of the same continuum model at all scales with the primary barrier to simulation being computing resources. The second category of multiscale problems encompasses applications where detailed physics at the atomistic or molecular level must be simulated to resolve the small scales, but the effect on and coupling to the continuum level is frequently unclear. We believe these two canonical categories span an important subset of DOE/SC applications of interest.

Today, current approaches to multiscale problems often involve *ad hoc* modeling assumptions, incomplete mathematical formulations, and numerical implementations that are inconsistent with both the mathematical and physical properties of the system. In general, multiscale research efforts remain largely disjoint across disciplines and typically focus on only one of the two multiscale categories. For example, in homogenization [16], heterogeneous multiscale [7], and some quasicontinuum methods [18], small scales are subordinate to a conventional coarse-grain model and serve to replace empirical closures by more accurate estimation procedures. Likewise, *ab initio* molecular, atomistic and particle modeling approaches [1, 8] focus on small scale interactions and less on their interface with coarse-grain models.

In contrast, the key mathematical and physical issues arising in multiscale problems: scale rep-

resentation, scale separation, and inter-scale communication; are common, and occur across a wide range of scientific disciplines. Consequently, there is a real and existing need for a mathematical framework that unifies these common principles and helps to analyze multiscale problems in a rigorous and systematic way.

A framework for multiscale analysis can identify and correct *ad hoc* assumptions and inconsistencies, and lead to a common mathematical formalism and structure to describe multiscale problems across multiple scientific disciplines. The variational multiscale method (VMS) of Hughes et al. [10] appears to be an especially promising foundation for a unifying multi-disciplinary mathematical formalism. VMS can provide the needed mathematical rigor and level of abstraction in dealing with issues common to multiscale problems such as scale representation, scale separation, and interscale communication.

A key element in extending VMS to address these issues is the formulation of generalized transfer operators for interscale communication that encompass the ideas of projection, subgrid modeling, and information creation/destruction at generalized scale interfaces. This formalism enables exploration of important issues in a general setting that is readily applicable to an extensive class of problems in fluid dynamics, reacting flows, geophysical flows, MHD, plasma systems, shock hydrodynamics, solid mechanics, materials science and biological systems that are relevant to DOE Office of Science applications. Such an effort is particularly timely both because of theoretical advances and the availability of large-scale computing platforms.

The viability of such an overarching new approach can be assessed by focusing initially on problems that exemplify the challenges facing multiscale science and engineering. Lab-centric, prototype application problems in fluid mechanics, shock hydrodynamics/plasma MHD and materials science are an important subset of DOE Office of Science applications and can serve as an ideal proving ground for this purpose.

In the following, we have selected three application areas from this subset that illustrate both the challenges and the potential payoffs from the new VMS framework, and that span both categories of multiscale problems.

- **Fluid Dynamics and Reacting Flows:** the framework can be applied to model turbulent transport and interface dynamics arising in a wide range of fluid systems. Important applications include turbulent fluid flow, combustion systems and general transport/reaction systems. This application area is representative of the category of problems where large and small scales are governed by the same PDE set, but where direct simulation demands tremendous computational resources. Additionally the turbulent reacting flow problem is an example where chemical species mixing, non-equilibrium chemical reactions, heat release and volumetric expansion occur at the small scales. As a result physical mechanisms in combustion are dominated by small scales and strongly interact and often drive large scales. Therefore mathematical models that do not correctly capture the complex small scale dynamics will be unsuccessful.

- **Materials Science:** the framework can be applied to model complex materials science problems that exhibit interactions ranging from continuum to nanoscales such as MEMS systems, fracture, crack propagation, and material fatigue. The range of scales and their interaction in these problems demands a coupled atomistic/continuum approximation. This application area highlights issues specific to the second category of multiscale problems, specifically, interfaces for coupling and interaction between qualitatively different models operating at vastly different length and time scales.

- **Shock Hydrodynamics/Plasma MHD Applications:** the framework can also be applied to model complex material behavior in the context of plasma systems and strong shocks for high energy deposition systems. Important DOE/SC applications in this area include the simulation of complex materials under high strain-rates, coupled plasma-hydrodynamic processes, and MHD turbulence. These applications exhibit features of both categories of multiscale problems requiring modeling of unresolved scales, bi-directional interscale coupling and interaction between different models that will exercise multiple facets of the interscale transfer mechanisms.

2 A Perspective on two Illustrative Multiscale Applications

In this section we offer a brief overview of current approaches to multiscale modeling as applied to the first two prototypical application areas identified above. The extant work is representative of both the type of ideas applied to multiscale problems and their limitations. Other target problems share features of these examples, but we note in passing that multiscale efforts in the third application area has been limited.

Fluid Turbulence

The predictive numerical modeling of fluid turbulence, even in non-reacting systems, remains an unsolved scientific problem. Turbulence simulation has traditionally taken one of three routes: Direct Numerical Simulation (DNS) where all scales in space and time are resolved, Large Eddy Simulation (LES) where only the large scales are represented, and Reynolds Averaged Navier–Stokes (RANS) where all turbulent motions are modeled and only the mean flow is predicted. Usually DNS and LES are too computationally expensive for complex large-scale analysis while RANS often has insufficient accuracy and reliability.

Pressured by the need to predict the largest scales of turbulent motions, there have recently been a number of efforts that attempt to merge RANS with LES in an effort to achieve an efficient multiscale simulation capability. These methods go by a variety of names including: Very Large-Eddy Simulation (VLES), Unsteady Reynolds Averaged Navier–Stokes (URANS), and Detached Eddy Simulation (DES) (see *e.g.*, Refs. [2, 14, 19–21, 24]).

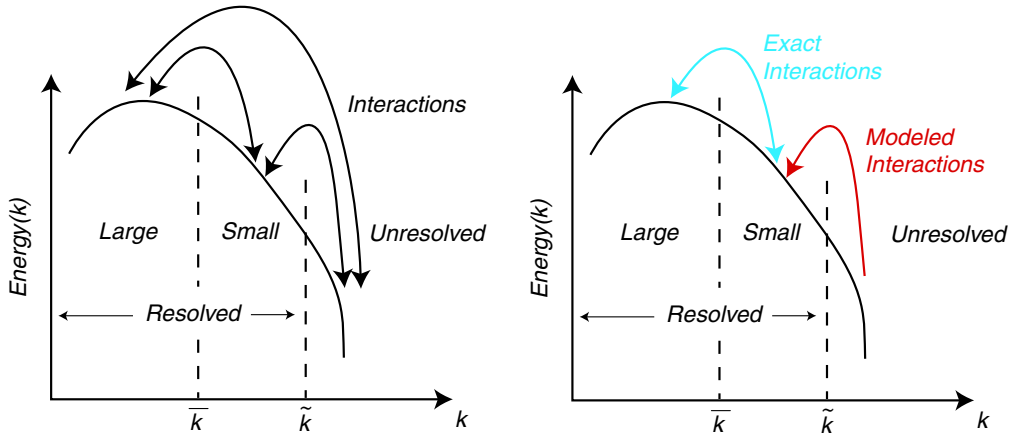

Figure 1. Schematic of interscale transfers in VMS modeling of turbulence. Left: no model, Right: model.

However, all these approaches, to varying degrees, are unsatisfactory for the following reasons: 1) The models are often developed and tuned for mean-flow solutions. 2) The models are typically developed with little regard to discretization errors. 3) Solutions do not converge in any meaningful way to the exact solution (DNS). 4) Ad hoc modeling techniques may be used such as blending functions between RANS regions and LES regions. 5) Spatial filters are often required that present difficulties for flows in complex geometries using unstructured meshes and for flows near boundaries. 6) Complex subgrid scale models may be used that can limit computational efficiency. And, 7) many models introduce effects across all the relevant scales (e.g. dissipation effects are introduced in both the large, supposedly resolved scales, as well as the small unresolved scales). In general these methods have scale separation characteristics that are difficult to characterize rigorously.

Recently, the Variational Multiscale approach to LES has been introduced (Hughes et al. [10]) that resolves many of the issues raised above for traditional RANS and LES. In particular, the VMS formulation provides a solid mathematical foundation for turbulence modeling where the extension to complex geometries is free from the issues related to commutativity and homogeneity that arise when using traditional spatial filters. Likewise, VMS allows for the "surgical" application of subgrid-scale models to model specific scale-to-scale interactions; e.g., one approach is to apply models only to the smallest resolved scales in a simulation, leaving large scales unaffected by direct modeling approximations/errors. This approach is demonstrated in Figure 1, which shows the potential inter-scale interactions in both a full DNS representation and in a VMS-LES model. The key modeling assumptions in this approach are discuss by Hughes et al. [10] and Collis [5]. By leaving the large scales untainted by direct modeling, VMS-LES has been shown to be more accurate than traditional LES methods for isotropic turbulence [11], wall bounded turbulence [12, 15], and even for controlled turbulent flows [17].

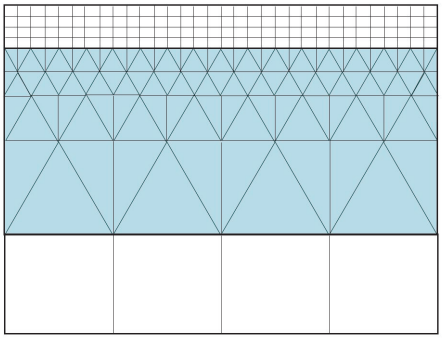

Figure 2. Overlap region in a coupled FE-MD model

Materials Modeling

Nearly all of the most difficult problems in solid mechanics, including the essential one of predicting material failure, involve the localization of the deformation to scales that are too small for the application of standard continuum models. Instead, the physics is dominated by interactions at the atomic or molecular scale, which are in turn strongly coupled to the macroscale deformation and stress fields. Although many *ad hoc* continuum models have been developed to try to capture these atomic scale effects, with varying levels of success, true understanding and accurate prediction of these phenomena for complex problems require computational techniques that couple continuum descriptions of materials with localized atomistic treatments.

One attempt to achieve this coupling is the Quasicontinuum Method [13], in which deformation fields are represented through interpolation among a selected subset of atoms. Adaptivity criteria are used to refine the interpolation in regions of high deformation, to the point where all atoms are represented where necessary. A major shortcoming of this approach is that it has only been developed for quasi-static problems at zero temperature. A method that can be used for dynamics is that introduced by Broughton et al. [4] for coupling finite elements (FE), classical molecular dynamics (MD), and tight binding (TB) quantum calculations in a single simulation of brittle fracture. In this technique, the finite element and molecular dynamics regions are coupled in an overlap region in which every atom in the MD simulation has a corresponding node in the FE mesh; see Figure 2. The result is an extremely fine FE mesh in the overlap region, which complicates meshing and adaptivity, increases computational expense, and limits the stable time step size that can be used for explicit time integration in the FE simulation. Fine scale energy in the MD simulation passes directly into the FE region, where it is subject to the dispersion errors inherent in a sharply graded mesh.

Recently, a bridging-scale coupling method was developed by Wagner and Liu [22] in which the coarse FE solution exists everywhere, while the MD simulation is used in localized regions without a need for node-to-atom matching. This method shares many characteristics with VMS as presented for the fluids turbulence modeling described above, and in fact can be reformulated

as a VMS system of equations. In this method a decomposition of the solution space by a special projection was used that partitioned the large scale and small scale kinetic energy contribution as a direct sum. Boundary conditions on the MD region allow fine-scale energy to pass cleanly out of the MD simulation. However, no satisfactory technique has yet been found for the treatment of this fine scale energy (perhaps as a temperature) in the FE-only region, nor is it understood how fine-scale information (e.g. fluctuations) should be created and introduced into the MD simulation at the boundaries. Scales are separated both in wavenumber and physical space, and a consistent mathematical treatment is needed to understand the correct interaction of these scale regions.

3 Mathematical Framework

This section begins with a very brief review of the Variational Multiscale (VMS) method that serves to form the foundation of our mathematical framework. With this background, we then discuss the important issues of identifying multiscale problems, scale representation/separation, and modeling interscale coupling.

Variational Multiscale (VMS) Method

Initial applications of VMS focused on problems where there exist one global scale of interest; see Hughes [9]. VMS has also been used to extract a model for the *unresolved* scales so as to provide a correction term for the resolved scales. Likewise, VMS [10] and related methods [6], have also been applied with good success to help model and improve the understanding of large eddy simulation (LES) for turbulent flows (see e.g., Refs. [5, 11, 12, 17]). The success and versatility of VMS indicates a unifying potential for the purposes of multiscale applications.

In VMS, the solution spaces are partitioned as a direct sum with the definition of an appropriate projection operator. The solution is then represented as $U = \overline{U} + U'$ where $\overline{U}$ are the large scales and U' are the small scales. As an example, consider each scale as a range of Fourier modes in wavespace (as shown in Figure 1), although other bases may be used in practice. One can readily derive the *exact* equations of motion for each scale range and appropriate modeling assumptions can be introduced for each equation (see Refs. [5, 10] in the context of LES).

Formally, the discrete, *modeled* equation takes the form

$$B(W,U)_\Omega = \overline{M}(\overline{W},U)_\Omega + M'(W',U)_\Omega + \overline{F}(\overline{W},U,U_b)_{\partial\Omega} + F'(W',U,U_b)_{\partial\Omega} \qquad \forall W \in \mathcal{V}$$

where $B(W,U)$ denotes the standard Galerkin variational operator, $\overline{M}$ and M' denote subgrid scale model terms acting on the large and small scales, respectively; $\overline{F}$ and F' are modeled flux terms integrated over the boundary of the domain; and U_b are prescribed boundary values. In this formalism, the model terms, $\overline{M}$ and M', replace interscale transfer operators[1] that explicitly depend

[1] These are the Reynolds and cross stresses in turbulent fluid flows

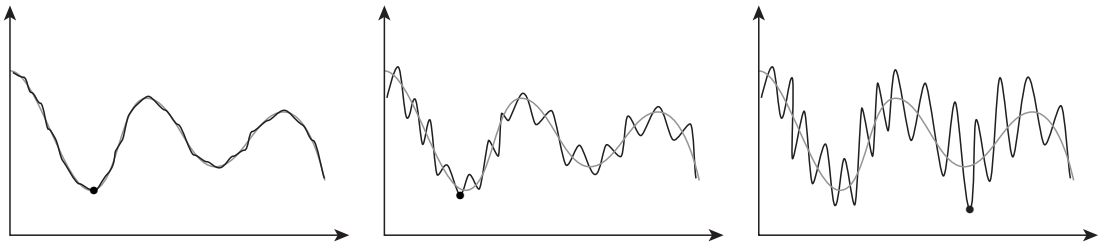

Figure 3. Two-scale energy landscape. Left: scale-uncoupled; Middle: scale-coupled; Right: scales-hopelessly-coupled. The ground state is denoted by • .

on unresolved scales of motion (i.e. subgrid scales). Likewise, the model flux terms also replace interscale transfer operators that represent the flux of unresolved scales across the boundary of the domain. These modeled flux terms provide a means for the transfer of multiscale information from outside the domain (through U_b) to the interior of the domain (see §3 for additional discussion).

The VMS framework allows one to readily identify scale-to-scale interactions and to surgically replace those interactions that depend on unresolved physics by appropriate model terms. Theoretical properties of the interaction of modeling assumptions on the various scales can be developed by use of the variational equations, the properties of the spaces and the associated projection operators. Of course, the particular choice of basis functions used to represent the solutions as well as the number and partitioning of this basis are important numerical algorithmic design issues that are discussed in more detail below. However, before doing so, it is first useful to discuss what we mean by a "multiscale problem."

Problems with multiple scales vs. multiscale problems

In the computational modeling of multiscale systems it is important to discriminate between problems with multiple active scales and problems that require explicit multiscale modeling. We address such questions in the context of a simple atomistic system in some detail, we then present a summary table as a brief organizing principle for broader classes of problems.

In atomistic simulations of molecular motions, the correct ground state configuration of a molecule is given by the solution to a global minimization. However, these physical systems operate within a multiscale energy landscape. The larger scales approximately correspond to modes of collective behavior at different groupings of their sub-scale modes. As a simple example with two scales only, consider a small molecule that is a covalently bound small group of atoms. The molecule evolves by individual atomic motions as well as by rotations around certain bonds.[2]

[2]Rotations about bonds can be decomposed into individual atomic motions, but are retained as a convenient representation, because the physics of the problem identifies them as a preferred mode.

In this context, the energy landscape can be decomposed into two distinct scales: atomic motions (small scale) and torsional motions (large scale). When viewed in phase-space, the large-scale mode has a set of minima in the angular dimension, while oscillations of atoms about their idealized torsional representation serve as a sub-scale oscillation. This problem can occupy three regimes in the energetic/thermal space: scale-uncoupled, scale-coupled, and scales-hopelessly-coupled. Figure 3 shows a schematic of these three configurations and we consider each in turn.

To begin, postulate that bond stretching and bond angles are much stiffer then torsions. Then we can have thermally activated torsions with bonds and angles nearly completely rigid. In this case the scales are decoupled—the system finds a ground state in the torsional coordinate alone and the influence of the atomic vibrations can be averaged out. No modeling of the individual atomic motions is needed and the left frame of Figure 3 represents this case.

Now, reduce the bond-stretching and bond-bending potentials to the point where the fluctuations in these quantities contributes to the determination of the ground state. This happens when fluctuations in the small-scale degree of freedom are on the order of the distinction between the metastable states in the larger (torsion) coordinate. Specifically, imagine that a particular torsional angle is favored because the atoms can assume the best bond-length. In this case, the scales are coupled and the small-scale needs to be modeled explicitly, although the larger scale remains a convenient representation and needs to be retained for efficiency. This is the scenario represented by the middle frame of Figure 3 where the inclusion of small-scale interactions leads to a slight, but important change in the ground state. In this case, inclusion of small-scale effects through some form of subgrid scale model is appropriate.

If the bond stretching and bending potentials are reduced even further, then the collective description of the torsion begins to lose meaning. The fluctuation in the torsional degree of freedom becomes so large that the individual scales are no longer distinct. This case requires explicit solution at the smallest scale since no purpose is served by collective representation. The right frame of Figure 3 represents this case where the inclusion of small-scale interactions leads to a radical change in the ground state.

While this example has been cast in the context of statics, conceptually, dynamical systems operate on a similar free energy landscape where the kinetic-energy barriers in different scales determine time-scales of collective modes.

To conclude this discussion, Table 1 summarizes the relationship between several essential properties of multiscale systems (scale-to-scale coupling strength, scale separation, and the length-scale of the driving mechanism) in order to highlight situations when coupled, multiscale modeling are required. A more complete description of this relationship is beyond the scope of the current discussion.

<table>
<tr><td colspan="2" rowspan="2"></td><td colspan="2">Driving Scale</td></tr>
<tr><td>Small</td><td>Large</td></tr>
<tr><td rowspan="4">Scale Interaction Strength</td><td>Strong</td><td>Multiscale
e.g. Combustion processes, coupled rigid body problems, Torsional dynamics of molecules, ….</td><td>Multiscale
e.g. Fluid turbulence with discontinuous boundaries and/or initial conditions etc., Crack propagation, ….</td></tr>
<tr><td rowspan="3">Weak</td><td>Scale Separation Details are critical</td><td rowspan="3">Homogenization, Heterogeneous Multiscale,
Quasi-continuum
e.g. porous media flow systems, linear elasticity with constitutive models, ..</td></tr>
<tr><td>Narrow: Multiscale
e.g. polymer physics, protein folding, ….</td></tr>
<tr><td>Wide: Atomistic, Molecular, etc.
e.g. ideal gases, hard single sphere interactions,</td></tr>
</table>

Table 1. Notional matrix of applicability of multiscale mathematical framework for coupled problems.

Scale Representation/Separation

As alluded to above, the VMS framework allows one to identify and model scale-to-scale interactions. However, before doing so, one must first select a basis with which to represent the solution (scale representation) and then decide how to separate or partition this basis in such a way that important scale ranges are identified and modeled in an appropriate manner.

Interscale coupling can be complex. How complex often depends on the choice of the basis. In our previous example (see §3), torsions were chosen in order to decouple the scales under common circumstances. Much of theoretical physics development owes its progress to just such choices, where a clever collective mode is identified that reduces interscale coupling, and thus simplifies the problem. However, for many problems, such a separation strategy is not obvious or may not even exist.

The last distinction can be critical: is the separation strategy hidden or simply does not exist? We would like to formulate an approach that would reveal the difference. For example, the choice of a Fourier basis has been found particularly useful in *periodic* systems, where *periodic* basis functions conform to the shape of the problem. However, a Fourier basis is known to produce unsolvable difficulties near non-periodic discontinuities. In those regions, scales couple strongly, producing undesirable artifacts. Numerous wavelet approaches have been invented that group scales (and wave numbers) in order to better represent localized features. An attractive quantitative approach is to use Renormalization Group (RNG) methods as a systematic approach to the multiple scale resolution

and coupling problem. The method was formalized for the 2-D Ising model by Wilson [23]. We wish to build on this foundation in order to understand the scale separation and representation issues inherent in a number of difficult multiscale applications.

Once a discrete basis is selected, how does one measure its quality? In a numerical simulation, we can test such issues by exciting each discrete mode and recording its dispersion relation into all other modes. The coupling constants form a weighted graph of connectivity between modes, cast as graph nodes. Such a graph can be analyzed for existence of components. If the graph partitions nicely into clusters, that are sparsely, or not at all, connected to each other, we have an excellent choice of basis, where individual scale divisions have been defined by the partition.

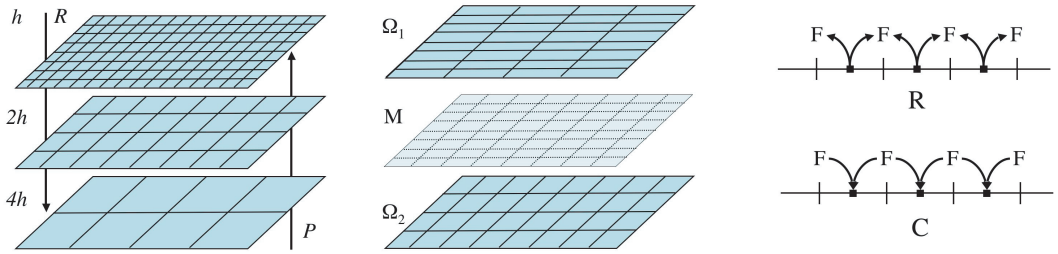

Figure 4. Examples of interscale communications: multigrid, mortar space and conservative finite difference methods.

Interscale Communication

How is information communicated across scales? In general this communication occurs at an interface that may be either in physical-space or in scale-space. Critical issues include how information is compressed and created at the interface. Existing methods such as multigrid, mortar finite elements, domain decomposition and conservation laws provide important examples of interface operators and regions; see Figure 4. In geometric multilevel methods, transfer of information occurs between grids with different spatial resolutions by virtue of restriction and prolongation operators. A relevant example are algebraic multilevel methods where scale separation and interscale transfer are effected by using the matrix graph. Note that in principle, this process is not dissimilar to the process suggested in the last section for assessing the strength of scale couplings; indeed, *aggregation* in algebraic multilevel methods follows essentially the same idea of edge clustering. This idea is shown graphically in Figure 5.

An example of a functional interface is provided by mortar elements that glue together disjoint approximations occupying different regions is space. Domain decomposition methods are another important prototype where interface communication is effected by Poincare-Steklov operators at the variational level and by the Schur complement at the algebraic level.

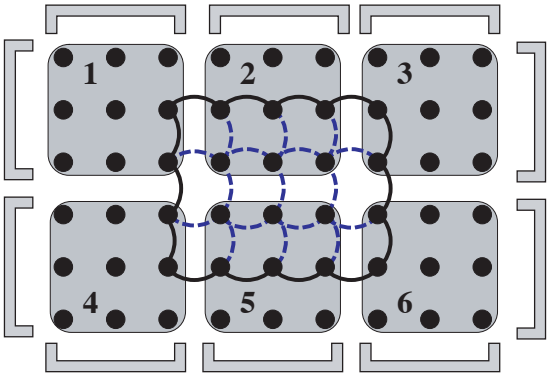

Figure 5. Aggregation in algebraic multilevel methods [3].

These examples encompass a range of ideas that may prove useful in the design of interscale communication operators. For instance, the compression/creation process at an interface is similar to finding an appropriate numerical flux, or creating the proper *mortar* space. The *flux* analogy seems especially appropriate in the light of the close parallels between reconstruction and averaging operators and the creation/compression process. Ultimately, the design of these operators must be guided by the physics of the problem that sets the effective *dispersion relation* governing the transfer of information either in physical or wave space.

As an example, consider of the interface between RANS and LES in a turbulent flow simulation. If information is convecting from the LES to RANS then some form of compression or elimination of the small-scale information is required. However, if information flows from RANS to LES, then small-scale turbulent fluctuations must, somehow, be generated that have the correct statistical properties. An analogous situation exists with atomistic (or molecular) small scale physics interacting with large scale continuum models in materials

4 Summary

The state of research in multiscale science and engineering has progressed to the point where there is a definitive need for an overarching mathematical framework that unifies common principles across disciplines in a systematic and rigorous fashion. To this end, the variational multiscale method has been identified as a viable candidate for such a mathematical framework and, in fact, has already been demonstrated on problems spanning the two primary categories of multiscale problems discussed here. Additionally, the key mathematical and physical issues of scale representation, scale separation, and inter-scale communication have been pointed out and discussed. We believe that a sustained focus on these issues will provide a general mathematical framework for multiscale prob-

lems. Finally a broad set of applications that are relevant to the DOE Office of Science and that can provide the proving grounds for assessing a multiscale framework have been outlined. This document represents our initial thoughts on developing a mathematical framework for multiscale applications. As such, we expect that future versions of this document will build upon these ideas.

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